APPLICATION NO.	FILING DATE	FIRST NAMED INVENTOR	ATTORNEY DOCKET NO.	CONFIRMATION NO.
09/502,133	02/11/2000	Harold E. Helson	103544.131US2	4787

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WILMERHALE/BOSTON
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EXAMINER
JONES, HUGH M

ART UNIT	PAPER NUMBER
2128	

NOTIFICATION DATE	DELIVERY MODE
09/02/2009	ELECTRONIC

Please find below and/or attached an Office communication concerning this application or proceeding.

The time period for reply, if any, is set in the attached communication.

Notice of the Office communication was sent electronically on above-indicated "Notification Date" to the following e-mail address(es):

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	Application No.	Applicant(s)
Office Action Summary	09/502,133	HELSON, HAROLD E.
	Examiner	Art Unit	
	Hugh Jones	2128	

-- *The MAILING DATE of this communication appears on the cover sheet with the correspondence address* --

Period for Reply

A SHORTENED STATUTORY PERIOD FOR REPLY IS SET TO EXPIRE <u>3</u> MONTH(S) OR THIRTY (30) DAYS, WHICHEVER IS LONGER, FROM THE MAILING DATE OF THIS COMMUNICATION.
- Extensions of time may be available under the provisions of 37 CFR 1.136(a). In no event, however, may a reply be timely filed after SIX (6) MONTHS from the mailing date of this communication.
- If NO period for reply is specified above, the maximum statutory period will apply and will expire SIX (6) MONTHS from the mailing date of this communication.
- Failure to reply within the set or extended period for reply will, by statute, cause the application to become ABANDONED (35 U.S.C. § 133).
  Any reply received by the Office later than three months after the mailing date of this communication, even if timely filed, may reduce any earned patent term adjustment. See 37 CFR 1.704(b).

Status

1) ☒ Responsive to communication(s) filed on <u>24 July 2009</u>.
2a) ☒ This action is **FINAL**.   2b) ☐ This action is non-final.
3) ☐ Since this application is in condition for allowance except for formal matters, prosecution as to the merits is closed in accordance with the practice under *Ex parte Quayle*, 1935 C.D. 11, 453 O.G. 213.

Disposition of Claims

4) ☒ Claim(s) <u>1,9 and 13-35</u> is/are pending in the application.
    4a) Of the above claim(s) _____ is/are withdrawn from consideration.
5) ☐ Claim(s) _____ is/are allowed.
6) ☒ Claim(s) <u>1, 9, 13-35</u> is/are rejected.
7) ☐ Claim(s) _____ is/are objected to.
8) ☐ Claim(s) _____ are subject to restriction and/or election requirement.

Application Papers

9) ☐ The specification is objected to by the Examiner.
10) ☒ The drawing(s) filed on <u>11 February 2000</u> is/are: a) ☒ accepted or b) ☐ objected to by the Examiner.
    Applicant may not request that any objection to the drawing(s) be held in abeyance. See 37 CFR 1.85(a).
    Replacement drawing sheet(s) including the correction is required if the drawing(s) is objected to. See 37 CFR 1.121(d).
11) ☐ The oath or declaration is objected to by the Examiner. Note the attached Office Action or form PTO-152.

Priority under 35 U.S.C. § 119

12) ☐ Acknowledgment is made of a claim for foreign priority under 35 U.S.C. § 119(a)-(d) or (f).
    a) ☐ All b) ☐ Some * c) ☐ None of:
        1. ☐ Certified copies of the priority documents have been received.
        2. ☐ Certified copies of the priority documents have been received in Application No. _____.
        3. ☐ Copies of the certified copies of the priority documents have been received in this National Stage application from the International Bureau (PCT Rule 17.2(a)).
    * See the attached detailed Office action for a list of the certified copies not received.

Attachment(s)

1) ☐ Notice of References Cited (PTO-892)
2) ☐ Notice of Draftsperson's Patent Drawing Review (PTO-948)
3) ☐ Information Disclosure Statement(s) (PTO/SB/08) Paper No(s)/Mail Date _____.

4) ☐ Interview Summary (PTO-413) Paper No(s)/Mail. Date _____.
5) ☐ Notice of Informal Patent Application
6) ☐ Other: _____.

DETAILED ACTION

1.   Claims 1, 9, 13-35 of U. S. Patent 09/502,133 are in front of the office for

consideration and remain pending. Claims 2-8, 10-12 are canceled.

Claim Rejections - 35 USC § 103

2.   The following is a quotation of 35 U.S.C. 103(a) which forms the basis for all

obviousness rejections set forth in this Office action:

> (a) A patent may not be obtained though the invention is not identically disclosed or described as set
> forth in section 102 of this title, if the differences between the subject matter sought to be patented and
> the prior art are such that the subject matter as a whole would have been obvious at the time the
> invention was made to a person having ordinary skill in the art to which said subject matter pertains.
> Patentability shall not be negatived by the manner in which the invention was made.

3.   The factual inquiries set forth in *Graham* **v.** *John Deere Co.*, 383 U.S. 1, 148

USPQ 459 (1966), that are applied for establishing a background for determining

obviousness under 35 U.S.C. 103(a) are summarized as follows:

1.   Determining the scope and contents of the prior art.
2.   Ascertaining the differences between the prior art and the claims at issue.
3.   Resolving the level of ordinary skill in the pertinent art.
4.   Considering objective evidence present in the application indicating
      obviousness or nonobviousness.

4.   Claims 1, 9, 13-35 are rejected under 35 U.S.C. 103(a) as being unpatentable

over Helson (The inventor's PhD thesis - of record) in view of Benecke et al.

(Applicant's IDS) and the taking of official notice.

5.   Helson discloses:

    identifying, from a connection table for a chemical

structure, an instance of chemical structural symmetry in the

chemical structure (pp, 145-149; fig. 4.5; chapter 4; fig. 3.5,

pg. 221, fig. 4.9, fig. 5.4);

    wherein the instance of symmetry includes symmetrically

equivalent atoms and bonds (page 246; fig. 4.5; chapter 4, fig.

4.9, 5.4);

    positioning atoms and bonds in the chemical structure

diagram pp. 145-149; page 246; fig. 4.5; chapter 3).

    Note page 203-211 (redrawing)
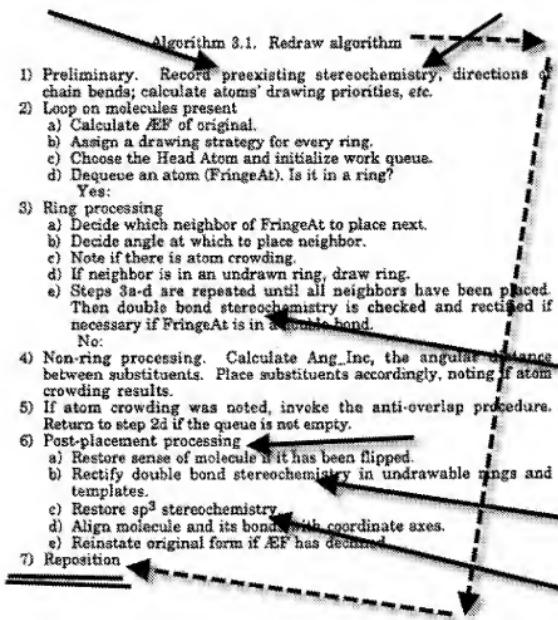
                                                                    204

                Table 3.1. Criteria for Aef_Redraw

        Criterion   Weight*   Description
            1   12   Bond overlap
            2   3   Bond alignment
            3   2   Angle alignment
            4   8   Bond distribution
            5   4   Alignment and zigzag of chains
            6   2   Alignment of ring bonds
            7   4   Macroorientation of ring systems
            8   6   Symmetry ◄
            9   8   Uniform bond length
           10   12   Atom crowding

*When a criterion is not applicable to a molecule its weight is set to zero.
 Similarly, the weights for criteria 5, 6 and 7 are adjusted to reflect the
 importance of the criterion to the molecule at hand.

    And (pg. 149):

Algorithm 3.1. Redraw algorithm

1) Preliminary. Record preexisting stereochemistry, directions of chain bends; calculate atoms' drawing priorities, etc.
2) Loop on molecules present
   a) Calculate ÆF of original.
   b) Assign a drawing strategy for every ring.
   c) Choose the Head Atom and initialize work queue.
   d) Dequeue an atom (FringeAt). Is it in a ring?
      Yes:
3) Ring processing
   a) Decide which neighbor of FringeAt to place next.
   b) Decide angle at which to place neighbor.
   c) Note if there is atom crowding.
   d) If neighbor is in an undrawn ring, draw ring.
   e) Steps 3a-d are repeated until all neighbors have been placed. Then double bond stereochemistry is checked and rectified if necessary if FringeAt is in a double bond.
      No:
4) Non-ring processing. Calculate Ang_Inc, the angular distance between substituents. Place substituents accordingly, noting if atom crowding results.
5) If atom crowding was noted, invoke the anti-overlap procedure. Return to step 2d if the queue is not empty.
6) Post-placement processing
   a) Restore sense of molecule if it has been flipped.
   b) Rectify double bond stereochemistry in undrawable rings and templates.
   c) Restore sp^3 stereochemistry.
   d) Align molecule and its bonds with coordinate axes.
   e) Reinstate original form if ÆF has declined.
7) Reposition

6.   Note that the redraw algorithm calls the **reposition algorithm**. See page 145-

146:

Implementation in CAMEO

In CAMEO, SDG is divided into two independent processes: SDG proper, referred to as "redrawing," and positioning of the resulting molecules, called "repositioning." Both facilities exist as independent packages of routines that may be called to serve different occasions; they are not rigidly tied to any particular phase of the program. In fact, repositioning does not even require perception, although redrawing does. The two executive

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routines are REDRAW for SDG proper, and ANA_REPO for positioning. At present REDRAW, which always invokes ANA_REPO at its end, is called from the following places:

Also see the table of contents:

7.   Helson does not appear to disclose

laying out atoms/bonds <u>to express the identified symmetry</u>

as previously argued by Applicants.

8.   Benecke et al. discloses laying out atoms/bonds to express the identified

symmetry (pg. 145):

> Each of the structural isomers may exist in several
> configurations in space. MOLGEN⁺ is capable of
> generating all possible configurational isomers, again
> redundancy free (which, of course, also implies the
> consideration of symmetries).
>
> The notion stereoisomerism is not uniquely de-
> fined in chemistry; it should therefore be stated
> which kinds of effects are taken into account. Pri-
> marily there are: (i) chirality of tetravalent atoms,
> even in rings and spiranes, and (ii) enantiomerism
> and diastereomerism of allenes including *cis/trans*-
> isomerism.

> The construction of the stereoisomers is per-
> formed in two steps: First the molecular graph is
> examined for stereochemical properties and the com-
> plete set of configurational isomers is generated
> without any use of three-dimensional information.
> This method is based on [6], improved by [9]. Table
> 2 shows the numbers of stereoisomers corresponding
> to all structural isomers of a single gross formula.

> In the second step spatial realizations of these
> isomers are calculated by the application of appropri-
> ate geometrical transformations to the placement
> computed above. (The basics of these calculations,
> which are again discussed in [7], can be found in
> [8].) In Fig. 2 the four stereoisomers of 1,2,3,4-tetra-
> methylcyclobutane are displayed as an example.

9.   It would have been obvious to one of ordinary skill in the art at the time of the

invention to so modify Helson in order to generate all configurations to facilitate

chemical research.

10.   As for dependent claims, Benecke et al. discloses (pg. 45):

> Each of the structural isomers may exist in several
> configurations in space. MOLGEN$^+$ is capable of
> generating all possible configurational isomers, again
> redundancy free (which, of course, also implies the
> consideration of symmetries).
>   The notion stereoisomerism is not uniquely de-
> fined in chemistry; it should therefore be stated
> which kinds of effects are taken into account. Pri-
> marily there are: (i) chirality of tetravalent atoms,
> even in rings and spiranes, and (ii) enantiomerism
> and diastereomerism of allenes including *cis/trans*-
> isomerism.

Official notice is taken that a skilled artisan would understand that there are a limited

group of possible symmetries and would employ them as appropriate. Also, see

(Helson) chapter 4 (examples of symmetry).

Response to Arguments

11.   Applicant's arguments, filed 7/24/2009, have been carefully considered and are

not persuasive.

12.   Process claims 1, 13-34 were analyzed under 35 USC 101. It is recognized that,

in order to be statutory, a process claim must be 1) tied to a particular machine or

apparatus, or 2) it transforms a particular article into a different state or thing. *In re*

Bilski, 88 USPQ2d 1385 (2008). It is also recognized that a general purpose computer

may be converted into a particular computer through the operation of software on the

computer. *In re Alappat*, 31 USPQ2d 1545 (1994). Claims 1, 28 (and with dependent

claims) recite in relevant part,


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"A computer-implemented method..."
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The process is therefore tied to a particular machine, and there are meaningful limits to

the claims, thus meeting the *Bilski* test. There is no transformation of matter. Medium

claims 9, 25 (and dependent claims) are also statutory. The claimed storage medium is

defined in the specification (second full par., pg. 20) to only refer to tangible physical

medium.

13.   Applicants argue (pg. 12):

> The Office Action refers to page 145 of Benecke, which states "MOLGEN is capable of generating all possible configurational isomers, again redundancy free (which also implies the consideration of symmetries)." This statement does not teach or suggest using symmetry to lay out atoms and bonds of a chemical structure in two-dimensional or three-dimensional space. Rather, symmetry is used to avoid redundancy in generating the listing of possible configurational isomers that satisfy the user-prescribed restrictions. By considering symmetry in creating these connection tables, redundancy is avoided. Nowhere does Benecke describe or suggest that the MOLGEN program use symmetry to determine how to lay out and position atoms and bonds in two-dimensional or three-dimensional space.

This constitutes a piecemeal analysis of the combination. The Benecke teaching was used to modify the Helson teaching, and must be viewed in that context. Regardless, Benecke also teaches (pg. 145):

> In the second step spatial realizations of these isomers are calculated by the application of appropriate geometrical transformations to the placement computed above. (The basics of these calculations, which are again discussed in [7], can be found in [8].) In Fig. 2 the four stereoisomers of 1,2,3,4-tetramethylcyclobutane are displayed as an example.

Note fig. 2. Whether this constitutes a 'structure diagram' or not is irrelevant.

14.   It is noted that removal of the 'redundancy' appears to be a natural by-product of identifying and expressing the symmetries, as claimed and as disclosed in the specification. Applicants are requested to explain their reasoning should they not agree. In any case, Applicants have not explained the nexus between 1) identifying the feature

and benefits of removing redundancy and 2) an alleged lack therefore of teaching the claimed invention. Regardless, the <u>inventor</u> (<u>Helson</u>) admits (pg. 13, arguments):

> Moreover, the consideration of symmetry in laying out atoms and bonds to create a chemical structure diagram was not contemplated at the time Benecke published. In a review article published in 1999, Helson includes symmetry as a "future advance" for structure diagram generation. Helson was aware of MOLGEN in that publication, as it is referenced (endnote 56, referenced from page 392). Thus, four years after publication of Benecke, persons of skill in the art still believed consideration of symmetry in producing chemical structure diagrams was a problem that had not been successfully solved.

Helson is stating that consideration of symmetry in laying out atoms and bonds to generate a structure diagram *was* contemplated in 1999.

15.   It is requested that Applicants provide a specific reference to the location in the 86 page Helson paper for the teaching regarding 'includes...symmetry as a 'future' advance..". This is extremely material as well as relevant to prosecution of the application.

16.   Applicants argue (pg. 12):

> atoms present and the valency of the atoms. (See, e.g., pages 142-143). The molecular graphs created by the MOLGEN program do not, in fact, include laying out atoms and bonds in a *chemical structure diagram*. For example, in the Abstract, Benecke explains that "*Afterwards* (i.e., after molecular graphs are produced) these molecular graphs can be displayed on the computer screen" (emphasis added).

The argument and patentable distinction is not clear.

17.   Claim 1 requires:

> 1. (previously presented) A computer-implemented method for use in deriving a chemical structure diagram, comprising:
>
> identifying, from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure;
>
> wherein the instance of symmetry includes symmetrically equivalent atoms and bonds;
>
> laying out symmetrically equivalent atoms and bonds in the chemical structure diagram to express the identified symmetry; and
>
> outputting a representation of the chemical structure.

It is noted that *laying out the symmetrically equivalent atoms and bonds* by itself means

that the symmetries are expressed.

18.   Referring again to the argument on pg. 13:

> Moreover, the consideration of symmetry in laying out atoms and bonds to create a chemical structure diagram was not contemplated at the time Benecke published. In a review article published in 1999, Helson includes symmetry as a "future advance" for structure diagram generation. Helson was aware of MOLGEN in that publication, as it is referenced (endnote 56, referenced from page 392). Thus, four years after publication of Benecke, persons of skill in the art still believed consideration of symmetry in producing chemical structure diagrams was a problem that had not been successfully solved.

The gist of the argument constitutes speculation. Furthermore, the speculation is based

upon the apparent opinion of Helson - *the instant inventor*. Furthermore, there is no

basis for the conclusion.

19.   Applicants are thanked for explaining the relevance of the identified documents

on pp. 7-9.

Conclusion

THIS ACTION IS MADE FINAL. Applicant is reminded of the extension of time

policy as set forth in 37 CFR 1.136(a).

A shortened statutory period for reply to this final action is set to expire THREE

MONTHS from the mailing date of this action. In the event a first reply is filed within

TWO MONTHS of the mailing date of this final action and the advisory action is not

mailed until after the end of the THREE-MONTH shortened statutory period, then the

shortened statutory period will expire on the date the advisory action is mailed, and any

extension fee pursuant to 37 CFR 1.136(a) will be calculated from the mailing date of

the advisory action. In no event, however, will the statutory period for reply expire later

than SIX MONTHS from the mailing date of this final action.

Any inquiry concerning this communication or earlier communications from the examiner

should be directed to Hugh Jones whose telephone number is (571) 272-3781. The examiner

can normally be reached on M-Th.

If attempts to reach the examiner by telephone are unsuccessful, the examiner's

supervisor, Kamini Shah can be reached on (571) 272-2279. The fax phone number for the

organization where this application or proceeding is assigned is 571-273-8300.

Information regarding the status of an application may be obtained from the Patent

Application Information Retrieval (PAIR) system. Status information for published applications

may be obtained from either Private PAIR or Public PAIR. Status information for unpublished

applications is available through Private PAIR only. For more information about the PAIR

system, see http://pair-direct.uspto.gov. Should you have questions on access to the Private

PAIR system, contact the Electronic Business Center (EBC) at 866-217-9197 (toll-free). If you

would like assistance from a USPTO Customer Service Representative or access to the

automated information system, call 800-786-9199 (IN USA OR CANADA) or 571-272-1000.

/Hugh   Jones/
Primary Examiner, Art Unit 2128